Uncertainty Analysis User's Manual

Symbolic Nuclear Analysis Package (SNAP)

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DAKOTA Uncertainty Plug-ins Users Manual

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Chapter 1. Introduction

The Symbolic Nuclear Analysis Package (SNAP) consists of a suite of integrated applications designed to simplify the process of performing thermal-hydraulic analysis. SNAP provides a highly flexible framework for creating and editing input for engineering analysis codes as well as extensive functionality for submitting, monitoring and interacting with the analysis codes. The modular plug-in design of the software allows functionality to be tailored to the specific requirements of each analysis code.

DAKOTA Uncertainty Analysis is provided as a SNAP plug-in. This plug-in provides a parametric job stream type and a job step that, when used together, perform uncertainty analysis. Both the stream type and plug-in leverage DAKOTA (Design Analysis Kit for Optimization and Terascale Applications), an open-source toolkit developed at Sandia National Laboratories. DAKOTA is used to generate random variates and to evaluate response data generated by an analysis code.

Resources for DAKOTA, including the lateI wst builds and User's Guides, are available at http://dakota.sandia.gov.

1.1. Uncertainty Analysis Approach

The general sequence of steps for performing an Uncertainty Analysis on a best-estimate model are outlined below:

1. Specify Uncertainty Analysis input such as sampling method, number of samples, etc.
2. Select the set of input parameters to be modified.
3. Assign probability distributions to each input parameter.
4. Generate the sets of random variates.
5. Generate an input file for each set of random variates.
6. Execute each case.
7. Extract response data from each case run.
8. Calculate uncertainty and sensitivity results.
9. Compile a report summarizing the Uncertainty Analysis.

The SNAP Uncertainty Analysis plug-in automates this process.

The first five steps are performed in the Model Editor prior to submitting the runs for execution. A DAKOTA Uncertainty Analysis parametric job stream is first created in a Job Stream enabled model. The configuration is defined as a property of the stream, including the selection of input parameters, definition and assignment of probability distributions, and input requirements given to the DAKOTA software such as the sampling method, number of samples, and the random seed.

When assembling the parametric tasks, each probability distribution function (PDF) produces one random variate per sampling iteration. The distribution specifies a

rule for how its random variates are applied to input parameters: each variate is treated as a replacement value, offset or coefficient. In addition, the PDF specifies its type (normal, log-normal, uniform, log-uniform, triangular, exponential, beta, gamma, Gumbel, Frechet, Weibull or histogram) and associated parameters (such as mean and standard deviation for a normal distribution). Certain distributions allow specifying optional range constraints that clip the range of values generated by the distribution. For example, normal distributions allow both an optional minimum and maximum, while uniform provides neither, as its only parameters are essentially bounds. The distributions are mapped to model variables; this distribution to variable mapping determines how the model is adjusted by the random samples.

In addition to defining the uncertainty configuration on the stream, it must utilize two custom stream steps to facilitate uncertainty analysis. The first, the AptPlot data extraction step, is used to pull the response data from the code results. The second handles running DAKOTA with the extracted results. Once both steps have been added and configured, the stream can be submitted.

When submitting the stream, a random sampling is made for each parametric task. The client uses DAKOTA to generate random variates for each probability distribution function. The variates are then applied to the identified input parameters and the input model is generated. Before exporting the model, a model check will be performed. Based on the uncertainty stream configuration, the input may be filtered out if it does not pass the model check without errors. Once the input is written or omitted, the modifications made to the model are reverted, and the next sample is taken (if more are required) or the complete input set is bundled for uncertainty stream execution.

During stream execution, the modified inputs are individually run through a user-defined sequence of stream steps; this can be as simple as a single code run or as complex as a chain of restarts that involves multiple analysis codes. The only requirement made by uncertainty is that the parametric sequence ends in a data extraction step: response data is pulled from plot files into a format understood by the DAKOTA Uncertainty step. This is where the AptPlot Extract Data step is applied: it executes a user-defined AptPlot script used to read the plot file, extract the appropriate response data, and write it to an ASCII file for later use.

After all of the cases have been executed and their response files have been generated, a parametric fan-in operation is performed to gather the results of each case to a common location. The uncertainty analysis step processes these individual response files to prepare an input file suitable for use by DAKOTA. Once the data is assembled, the DAKOTA executable is run with the generated input. The DAKOTA output will include confidence levels, response function probability distributions, and other properties the user has specified in the initial setup. After this step has run, a final report generation stage is executed in the stream.

The generated report summarizes the DAKOTA results and includes a description of results obtained from each of the individual calculations. The report will include a description of the modified parameters for each of the cases and identify which

runs completed successfully and which ones failed. Key metrics are provided for each response, such as a cumulative distribution function covering the entire result set. A summary of the uncertainty run configuration can also be provided; this summary covers the input parameters modified by the uncertainty run (along with their original values) linked to a description of the probability distribution function that provided the variations.

Chapter 2. Installation

Before uncertainty analysis can be performed, a DAKOTA executable must be installed in SNAP. On Windows systems, a DAKOTA binary is installed automatically by the plug-in installer. On other operating systems, you will need to install DAKOTA manually.

This section assumes that you have already installed the DAKOTA Uncertainty Analysis SNAP plug-in through the SNAP installer.

Installing DAKOTA

Follow these steps to install DAKOTA:

1. Create a `Dakota` folder in your SNAP installation directory. On most systems, the case for the folder name will have to match the indicated folder name exactly.

2. If you do not already have a DAKOTA binary for your system, download one from http://dakota.sandia.gov

3. Copy the DAKOTA binary into the `Dakota` folder as with one of the following names: `dakota.exe`, `dakota.sh` or simply `dakota`. Again, the filename will have to be completely lowercase on most systems.

   If you are using the Cygwin-dependent public release of DAKOTA for Windows, you may need to copy certain library files from the DAKOTA distribution `bin` folder into the SNAP `Dakota` folder. You can also copy the contents of the entire `bin` folder for simplicity.

4. Depending on your system, you may need to set executable permissions on the DAKOTA binary. Ask your local system administrator for more information about setting the appropriate permissions.

This places DAKOTA in a location where your local SNAP installation can invoke it to generate random variates.

DAKOTA Application Definition

Full use of the DAKOTA Uncertainty Analysis plug-in requires a DAKOTA application definition in your SNAP configuration. This application definition is added for you automatically, but will require adjustment if you had to install DAKOTA manually and did not use the file name `dakota`.

1. Open the Configuration Tool.
2. Expand the Applications list and select **DAKOTA**. The path specified in the Local Location for this application uses the ${SNAPINSTALL} keyword to indicate the location of your SNAP installation.

3. Adjust the path to reflect the correct file name of the DAKOTA executable.
4. Save the SNAP Configuration: either press the **Save** button in the toolbar or select **File** > **Save** from the main menu.

AptPlot Data Extraction

The Uncertainty Analysis plug-in provides a job stream step that uses AptPlot to extract data from plot files. Similar to DAKOTA, an Extract Data application definition will be created for you automatically. However, if you do not have AptPlot installed, or install it in a folder other than the default, you will need to follow these steps.

1. Install AptPlot. The AptPlot installer and installation instructions can always be found at http://www.aptplot.com.

2. Open the Configuration Tool.

3. Expand the Applications list and select **Extract Data**.

4. Set your Local Location as the path to either `AptBatch.exe` or `aptbatch.sh` in your AptPlot installation `bin` directory. If you installed AptPlot to the default directory, the default Local Location will usually be correct.

5. Save the SNAP Configuration: either press the **Save** button in the toolbar or select **File** > **Save** from the main menu.

Chapter 3. Uncertainty Stream Type

To start performing uncertainty analysis in SNAP, create a new job stream. When creating the stream, you will be prompted to select a stream type. Select **DAKOTA Uncertainty** from this list. This type of stream forms the foundation for uncertainty analysis in SNAP.

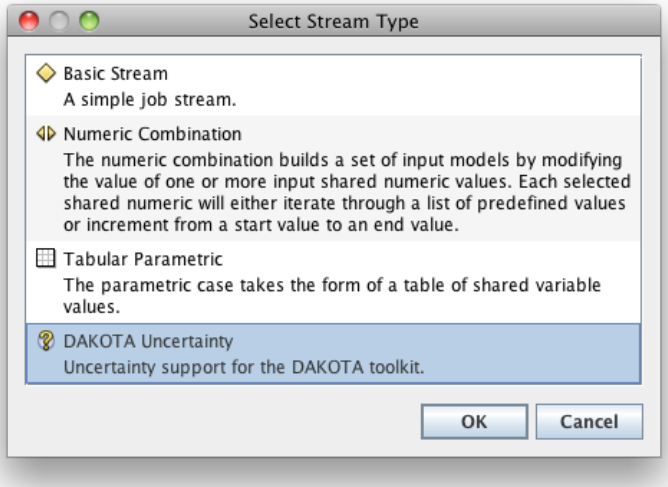

Select Stream Type
Basic Stream
A simple job stream.
Numeric Combination
The numeric combination builds a set of input models by modifying the value of one or more input shared numeric values. Each selected shared numeric will either iterate through a list of predefined values or increment from a start value to an end value.
Tabular Parametric
The parametric case takes the form of a table of shared variable values.
DAKOTA Uncertainty
Uncertainty support for the DAKOTA toolkit.
OK
Cancel

Figure 3.1. Select Stream Type Prompt

After creating the stream, you will need to edit the stream's DAKOTA configuration. This defines the basic structure of an uncertainty analysis, including how many random samples must be generated, what figures of merit must be examined, the probability distributions that define random variates applied to the model, and which random variates are mapped to which model variables.

The DAKOTA configuration is edited via the **Parametric Properties** attribute of the uncertainty stream. Editing this property opens the Edit Uncertainty Configuration window. The configuration is split across multiple tabs:

- DAKOTA Properties Tab - the high-level properties for the uncertainty analysis, such as sample count, figures of merit, and so on.
- Variables Tab - defines which model variables are mapped to probability distributions.
- Probability Distributions Tab - specifies the probability distributions that define the generated random variates.
- Report Configuration - configures the OpenDocument Format report generated by DAKOTA steps.

The **Undo** and **Redo** buttons at the bottom of the editor can be used to revert any changes made to the configuration since the editor was opened. This history is cleared when the editor is dismissed.

Press the **OK** button to accept the changes made to the configuration; if the configuration is invalid, a prompt will be displayed indicating the error. You can discard changes made in the editor at any time by either pressing the **Cancel** button or closing the window.

3.1. DAKOTA Properties Tab

The DAKOTA Properties panel implements the high-level properties for the uncertainty analysis.

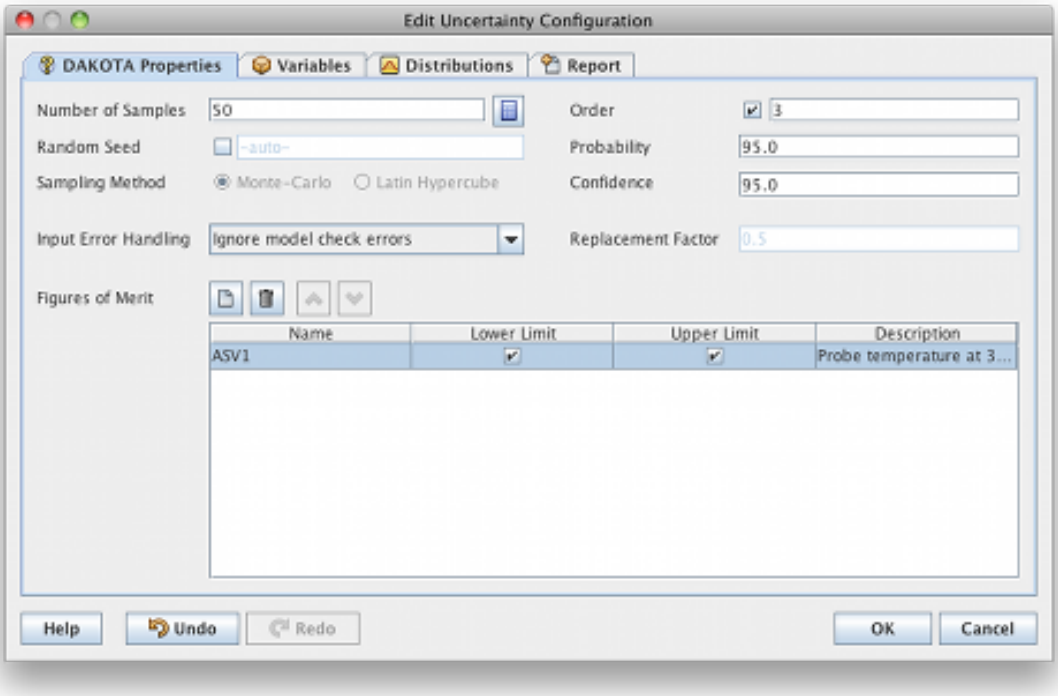


Figure 3.2. DAKOTA Basic Configuration

Set the **Number of Samples** to the number of random samplings applied to the model. The **Calculate Samples** button to the right of this field can be used to compute the required number of tasks for the indicated **Order** and **Probability** and **Confidence** intervals according to the Wilks method. This calculation is described in more detail in *Wilks Sample Computation*.

The **Random Seed** field can be used to override the seed used to generate pseudo-random numbers in DAKOTA. Select the check box and enter a value to specify an explicit seed. When set to a specific value, DAKOTA will generate the same sequence of values every time the stream is run. If left unset, DAKOTA will generate its own seed based on the current time.

Note Setting the seed will maintain a constant series of variates assuming the rest of the configuration remains the same. For example, changing the number or configuration of the probability distributions will change the generated values.

The **Sampling Method** specifies another constraint on random value generation. With Monte-Carlo, each random variate is produced from its distribution independent of other variates; a "good" spread of variates across the distribution is never guaranteed (although it is likely for a large number of samples). When set to Latin Hypercube, the distribution is sliced into equally likely *bins*, and a random value is produced from each bin. The number of bins is equal to the number of samples needed. By design, the Latin Hypercube method assures that the distribution will be more easily covered with fewer samples.

Note Activating the **Order** value indicates that the order statistic approach is being used. This disables the sampling method buttons after setting them to **Monte-Carlo**. See *Order Statistic Method* for more information.

Input Error Handling indicates how the uncertainty stream handles samples that cause a model to fail its model check. By default, model check errors are ignored and the sample is used regardless. The stream can also choose to simply filter out any samples that produce model check errors. The third option uses the **Replacement Factor** field to create substitutes for failed samples. When using the replacement strategy for an uncertainty stream with *n* samples and a replacement factor of *k*, the stream will generate a pool of $n+(k*n)$ inputs. Inputs are taken from this pool, filtering out inputs that fail model check with errors, until either *n* samples are selected or the pool is exhausted.

Figures of Merit

A figure-of-merit (FOM) is a single scalar value calculated from the results of a single analysis code run. The bulk of DAKOTA uncertainty analysis is oriented around analyzing and correlating FOM values across the parametric tasks (where each task represent a set of random samples). The **Figures of Merit** table is used to indicate which FOMs are expected for uncertainty analysis. The process of extracting the response values from the data is handled within the stream by the AptPlot Extract Data step (see AptPlot Data Extraction Step).

Note "Figure of merit" is approximately synonymous with the term "response function" found in DAKOTA literature.

Each FOM is defined by an upper and lower limit flag, used to compute the tolerance interval/limits from the response data. The FOM names and upper/lower limit flags are edited directly in the table. An uncertainty stream must specify at least one figure of merit.

Each FOM may also specify a description, which will be carried through to the report generated by DAKOTA Uncertainty steps (see DAKOTA Uncertainty Step). Editing the description displays an editing dialog, as shown in Figure 3.3.

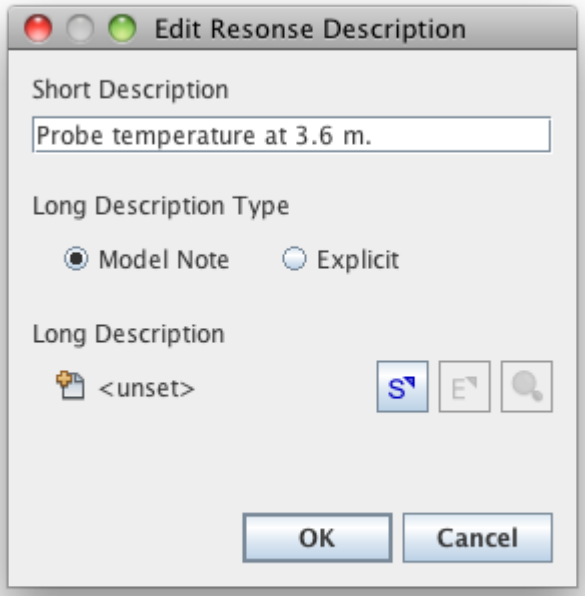


Figure 3.3. Description Dialog

There are two types of description: short and long. The short description is limited to 256 characters and will be shown most places the FOM is referenced, such as above tables listing the FOM data. Long descriptions may be edited as either an explicit block of text or as a reference to a model note. The long description is only displayed in the final section detailing DAKOTA-calculated results for the response, including its cumulative distribution function, mean, etc.

When Long Description Type is set to Model Note, a set of buttons appear used to edit the note reference. These buttons are, in order: selecting the note (the selection dialog can be used to create a new note), edit the referenced note, and create and display a preview of the note as an OpenDocument Format file. When set to Explicit, a text area appears in which to enter or edit the long description.

3.2. Variables Tab

Variable definitions control how the input model is varied for each set of random samples. This tab is composed of a central table, where model variables are mapped to probability distributions (see Probability Distributions Tab), and table controls used to add, remove, and reorder rows. The first two columns in the table indicate the name of the variable and the probability distribution it maps to. The remaining read-only columns indicate additional values of interest pulled from the referenced variable and probability distribution.

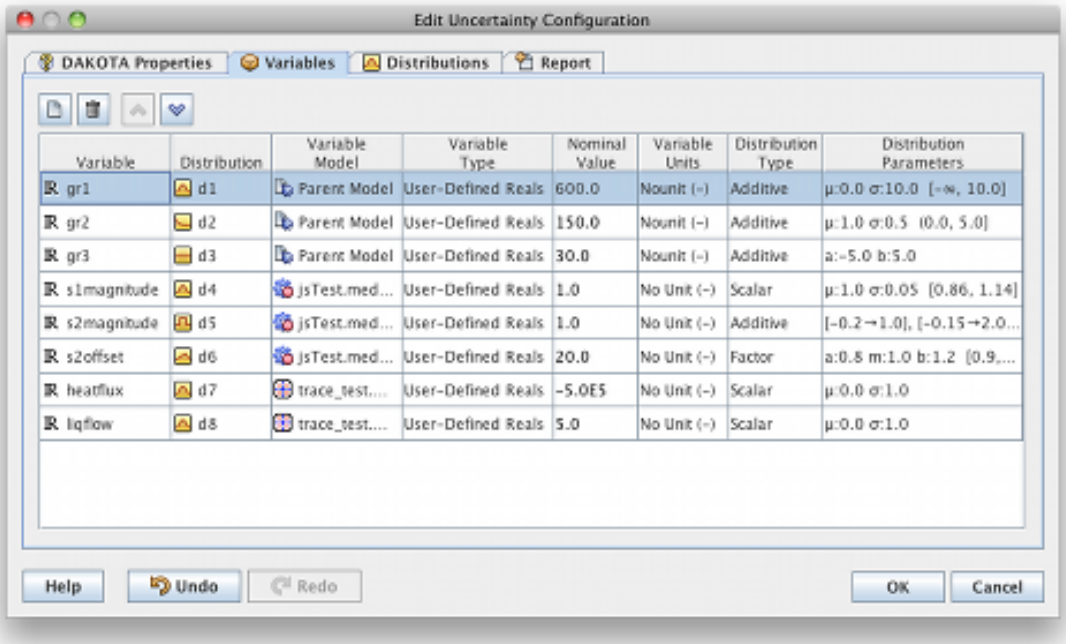

Edit Uncertainty Configuration
DAKOTA Properties
Variables
Distributions
Report
Variable
Distribution
Variable Model
Variable Type
Nominal Value
Variable Units
Distribution Type
Distribution Parameters
gr1 d1 Parent Model User-Defined Reals 600.0 Nounit (-) Additive μ:0.0 σ:10.0 [-∞, 10.0]
gr2 d2 Parent Model User-Defined Reals 150.0 Nounit (-) Additive μ:1.0 σ:0.5 [0.0, 5.0]
gr3 d3 Parent Model User-Defined Reals 30.0 Nounit (-) Additive a:-5.0 b:5.0
s1magnitude d4 jsTest.med... User-Defined Reals 1.0 No Unit (-) Scalar μ:1.0 σ:0.05 [0.86, 1.14]
s2magnitude d5 jsTest.med... User-Defined Reals 1.0 No Unit (-) Additive [-0.2→1.0], [-0.15→2.0...
s2offset d6 jsTest.med... User-Defined Reals 20.0 No Unit (-) Factor a:0.8 m:1.0 b:1.2 [0.9,...
heatflux d7 trace_test.... User-Defined Reals -5.0E5 No Unit (-) Scalar μ:0.0 σ:1.0
liqflow d8 trace_test.... User-Defined Reals 5.0 No Unit (-) Scalar μ:0.0 σ:1.0
Help
Undo
Redo
OK
Cancel

Figure 3.4. Model Variables Configuration

Note The **Variable Model** column only appears in Engineering Template models. This column indicates the source model for the indicated variable.

Creating a new variable reference opens a completion dialog, shown in Figure 3.5 and Figure 3.6. This process is broken into two steps. When selecting variables in an Engineering Template model, a combo box is displayed at the top of the dialog, used to select which model's variables are displayed. The tree on the left displays a hierarchy of available variable categories. This category hierarchy is entirely determined by the plug-in, though most will automatically support user-defined real numerics. The list on the right displays the model variables for the selected category. Once a model variable has been selected, the Next button can be used to move on to the second step.

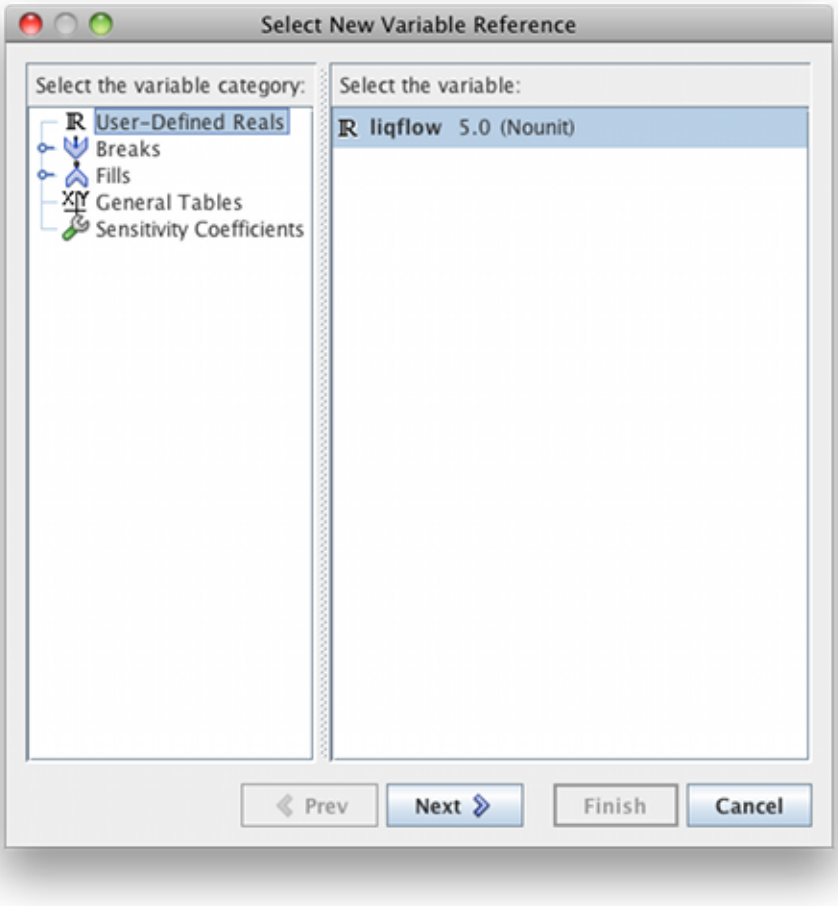


Figure 3.5. Referencing a model variable: Step 1

The second step is used to select or create a probability distribution for the reference. You can select or copy an existing distribution, or create a new distribution with one of the three variate application rules: Scalar, Additive and Factor. The figure below shows all available options; model variables may exclude certain application rules, which affects which choices are actually shown.

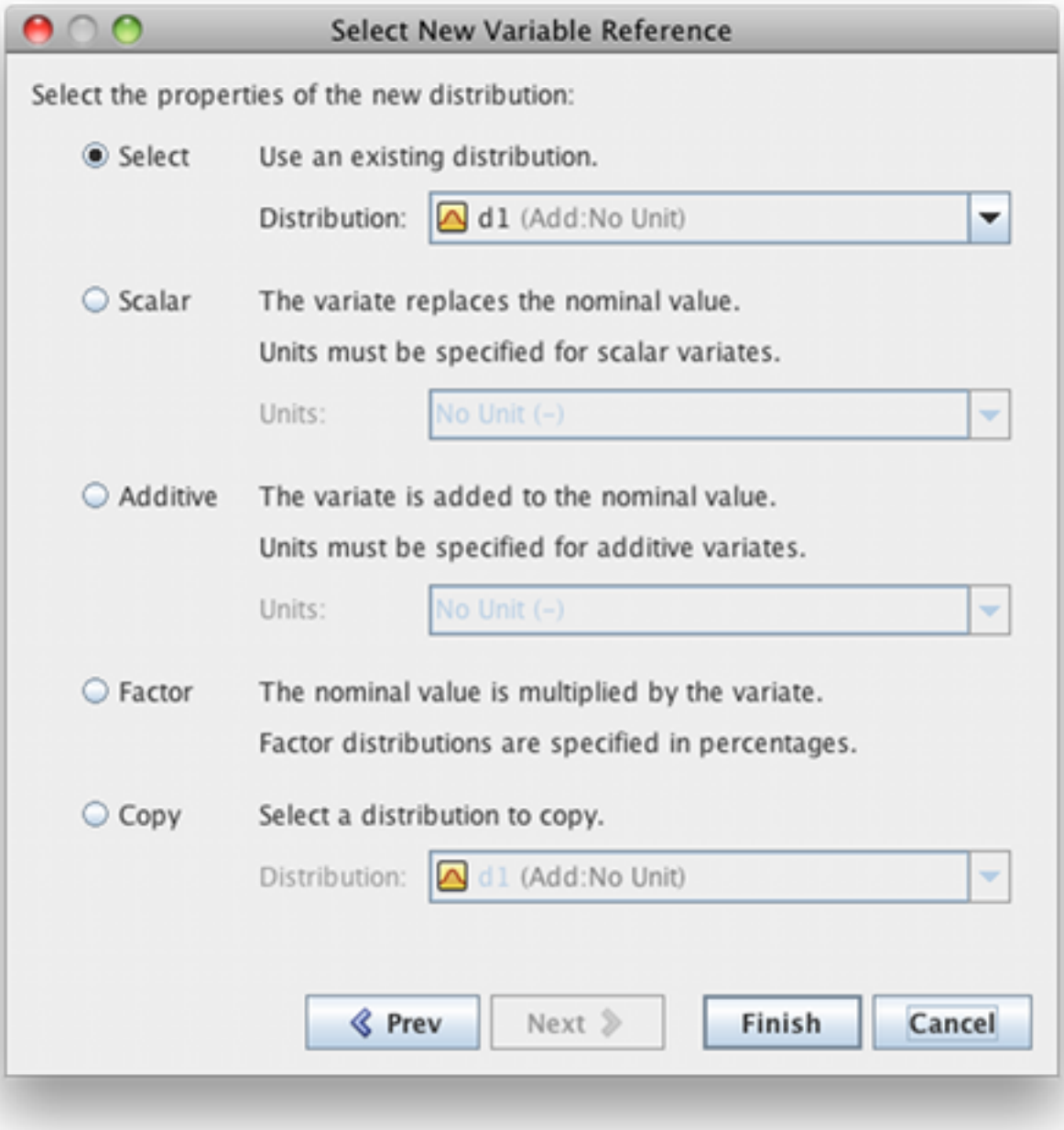


Figure 3.6. Reference a model variable: Step 2

The full list of options are as follows:

- **Select** - use a probability distribution that has already been defined. The list of available distributions will include all factor distributions and any scalar and additive distributions that have matching units. If the mapped variable does not allow a certain application rule, distributions of that type will not be listed.

- **Scalar** - create a new scalar distribution, where random variates replace the nominal value. When this value is selected, the Units drop-down indicates the units that may be applied to the model variable.

- **Additive** - create a new additive distribution, where random variates are added to the nominal value. Like Scalar, the units for Additive distributions must match the model variable. See the note below for more information on Additive distribution units.

- **Factor** - create a new factor distribution, where nominal values are multiplied by randoms variates. Factor distributions do not specify units and can be applied to any model variable.

- **Copy** - copy the selected distribution with a new name. The list of available distributions follows the same constraints as Select.

The descriptions for the distribution rules illustrate the general case for how random variates are applied to model variables based on the rule. Individual model variables may handle them differently, for example setting a mode flag based on the rule while always replacing the model variable with the variate.

Note Additive distributions will automatically use "difference" units for units with offsets in their conversion. For example, a "temperature difference" unit is used for temperature variables, where 1 degree Kelvin or Celsius is converted to 1.8 degrees Fahrenheit instead of -457.87 and 33.8, respectively. This keeps the amount added to the nominal value consistent regardless of the unit mode used in the model. Note that your Additive distribution must still be defined in the "base" units so that it matches the model variable.

Multiple variables can reference the same probability distribution if necessary. Selecting cells in the Distribution column displays an editor used to change the reference. Pressing the editor **Select** button opens a distribution selection dialog, as shown in Figure 3.7.

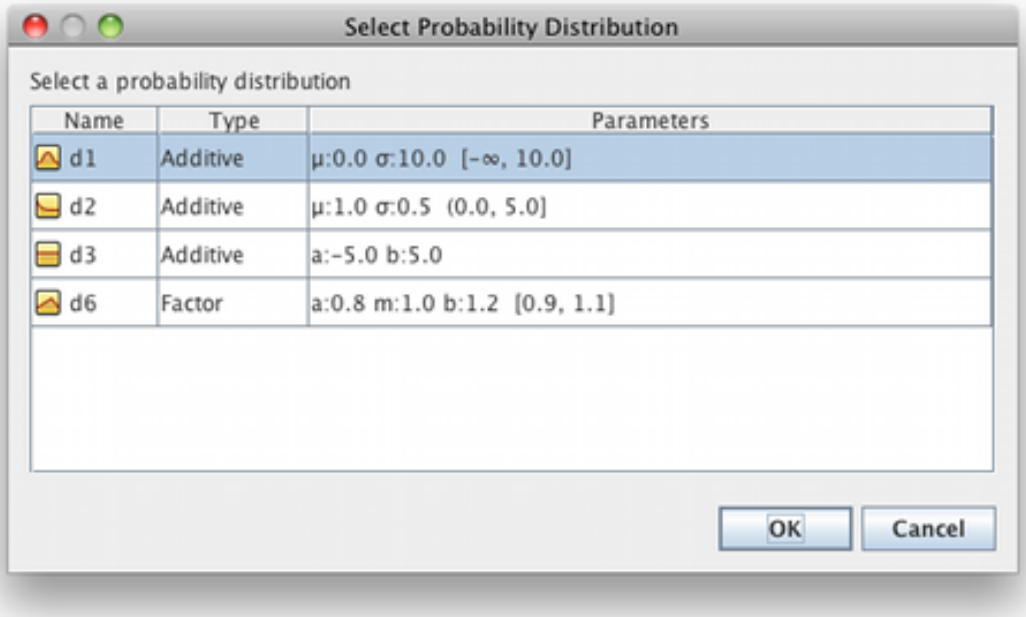


Figure 3.7. Selecting a probability distribution

One random variate is generated per probability distribution definition in each parametric task, allowing the user the flexibility to consistently apply a single variate across multiple values.

3.3. Probability Distributions Tab

The **Distributions** tab is used to specify the probability distributions that define random variate generation. Each probability distribution created in the dialog corresponds to exactly one random variate generated per parametric task.

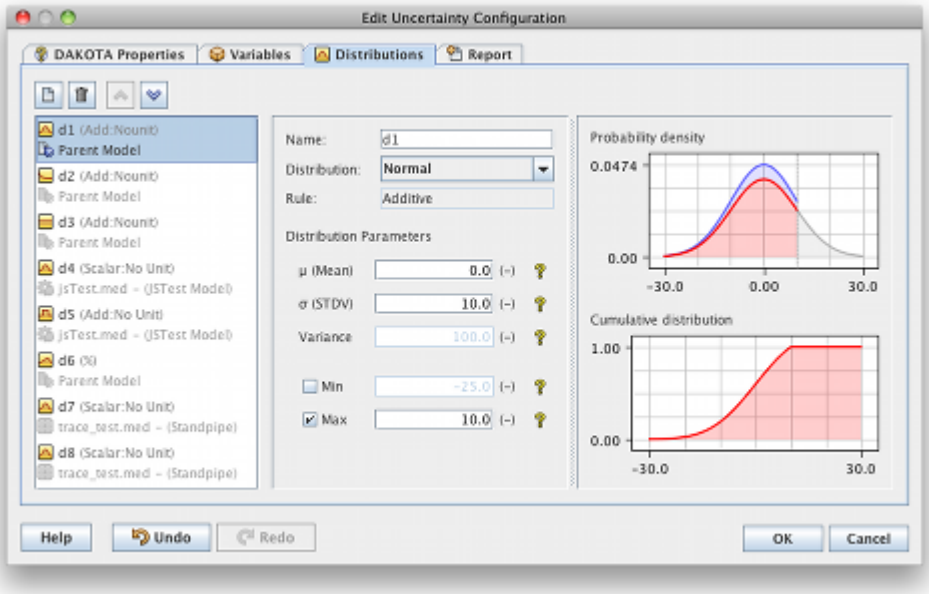


Figure 3.8. Editing the probability distributions

The list on the left shows the distribution. Select an item in the list to display its properties in the rest of the dialog. The central area is used to modify distribution properties, including name, type, and type-specific parameters. The uncertainty plug-in supports the following types of probability distribution: normal (Gaussian), log-normal, uniform, log-uniform, triangular, exponential, beta, gamma, Gumbel, Frechet, Weibull and histogram. Type-specific parameters are displayed in the Distribution Parameters section. Additionally, the right-most section of the tab displays a visualization of the probability distribution through its density and cumulative distribution functions. The graphs are updated as the distribution parameters are modified.

Note The icon next to each distribution is a direct indication of its type. Also, the model indicator shown in the distribution list only appears in Engineering Templates.

The normal, log-normal, and triangular distributions allow clipping a probability distribution via optional **Min** and **Max** fields. When the distribution is clipped, the skew applied to the unbound probability density function is displayed as a blue curve, with the clipped region shown in gray. The cumulative distribution curve is also adjusted for the clipped region, as shown in the figure.

New distribution definitions are specified as either a Factor, Additive, or Scalar distribution, which dictates how a generated random variate is applied to nominal values.

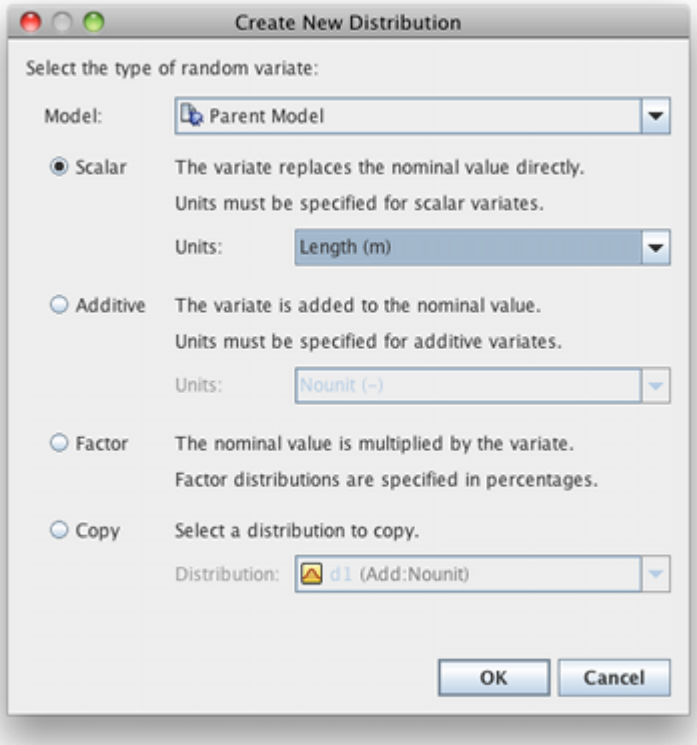


Figure 3.9. Creating a new probability distribution

The full list of options are as follows:

- **Model** - distributions in an Engineering Template model must also specify the model they apply to. Distributions can only be mapped to variables with matching models.

- **Scalar** - create a new scalar distribution, where the random variate replaces the nominal value. When this value is selected, the Units drop-down is used to select the units for the new distribution. Distributions may only be matched to model variables with matching units.

- **Additive** - create a new additive distribution, where the random variate is added to the nominal value. Like Scalar, the units for Additive distributions must be defined. See the note below for more information on Additive units.

- **Factor** - create a new factor distribution, where the random variate is multiplied against the nomainl value. Factor distributions can be applied to any model variable. Factor distributions are indicated with a percentage sign (%) next to their name.

- **Copy** - copy the selected distribution with a new name.

The descriptions for the distribution rules illustrate the general case for how random variates are applied to model variables based on the rule. Individual model variables may

handle them differently, for example setting a mode flag based on the rule while always replacing the model variable with the variate.

Note Additive distributions will automatically use "difference" units for units with offsets in their conversion. For example, a "temperature difference" unit is used for temperature variables, where 1 degree Kelvin or Celsius is converted to 1.8 degrees Fahrenheit instead of -457.87 and 33.8, respectively. This keeps the amount added to the nominal value consistent regardless of the unit mode used in the model. Note that your Additive distribution must still be defined in the "base" units for those model variables it will map to.

3.4. Report Configuration

The **Report** tab specifies properties of the report generated by a DAKOTA Uncertainty step (see DAKOTA Uncertainty Step).

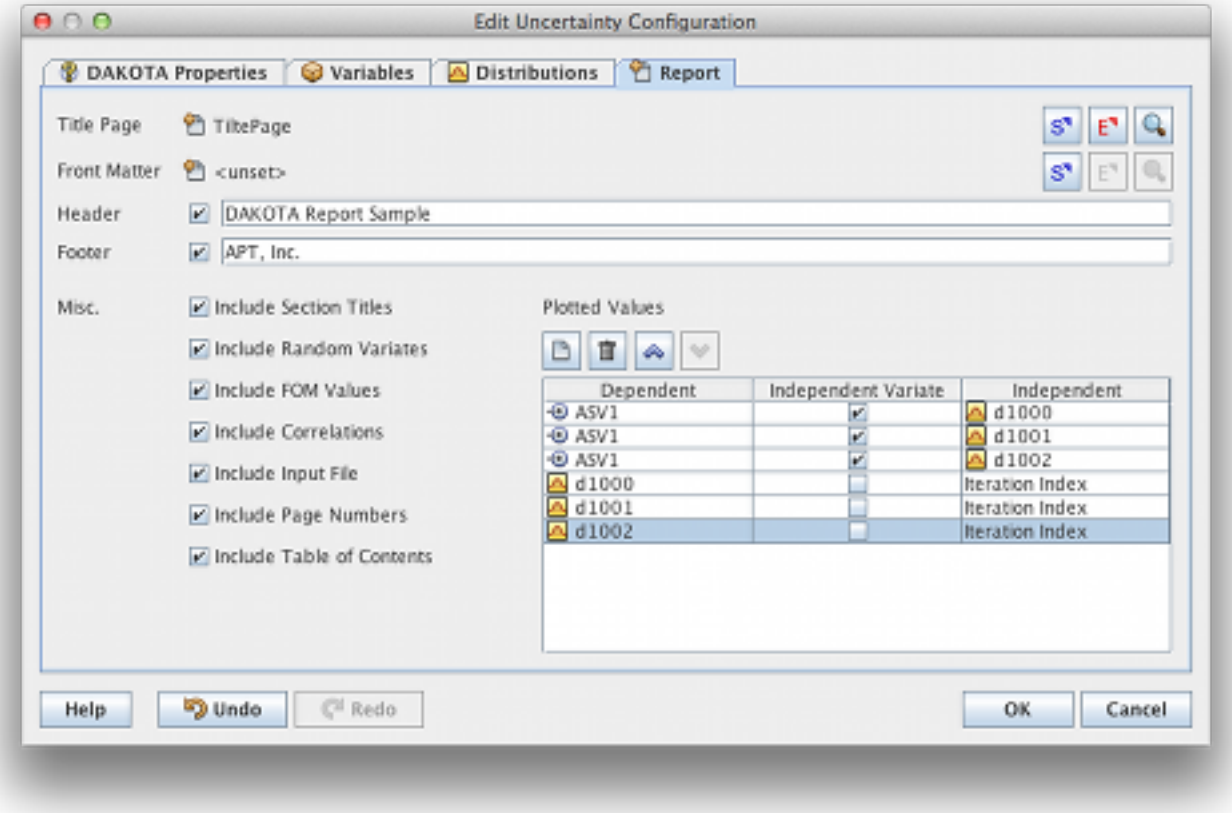


Figure 3.10. Editing the Report Configuration

Title Page allows setting a model note that will be used as the first page shown in the report. **Front Matter** is similar: the contents of the selected note will be displayed after the title page and table of contents. The buttons for both fields have the same functions. Press the blue **Select** button to select an existing note. Press the red **Edit** button to edit

the currently selected note. Press the **Preview Note** button to generate and display the note as an OpenDocument Format file.

The optional **Header** and **Footer** text provide optional labels to display at the top and bottom of each page in the document (except the title page). The **misc** section provides access to numerous features that are displayed in the document by default. The options are as follows:

- **Include Section Titles**. When enabled, a section title will be displayed in the header, listing the name of the top-level section on which the page begins.
- **Include Random Variates**. When enabled, every random variate generated for the uncertainty run will be listed in the report.
- **Include FOM Values.** When enabled, every FOM value result will be listed in the report. If both random variates and FOM values are included and the combined number of variates and FOMs is five or less, the results will be shown in a single table for convenience.
- **Include Correlations**. This option corresponds to the inclusion of correlations computed by DAKOTA. Correlations are broken down by response function and listed as a table of simple, partial, simple rank, and partial rank correlations relative to variates and other response functions.
- **Include Input File**. When enabled, the DAKOTA input file used to generate variates and perform the uncertainty analysis is written to the report.
- **Include Page Numbers**. When enabled, page numbers will be displayed in the document footer.
- **Include Table of Contents**. When enabled, a table of contents will be written to the report. This table is written as an OpenDocument Format construct that automatically adds entries whenever the document is updated.

The **Plotted Values** table can be used to include plots of figures of merit or random variate samples. Use the controls above the table to add, remove and reorder entries. Adding a row will display a completion dialog used to select the plotted data. By default, the values are plotted against the iteration index that each variate or response corresponds to. Alternatively, select the check-box in the **Use Independent** column to enable plotting against another FOM or distribution. Once enabled, use the cell editor in the **Independent** column to select the second set of data. FOM data can be plotted against distributions or other FOMs, and similarly distributions can be plotted against FOMs or other distributions.

Chapter 4. Job Stream Steps

Once the DAKOTA configuration for an uncertainty job stream is specified (see Chapter 3, *Uncertainty Stream Type*), you will need to add steps to the stream.

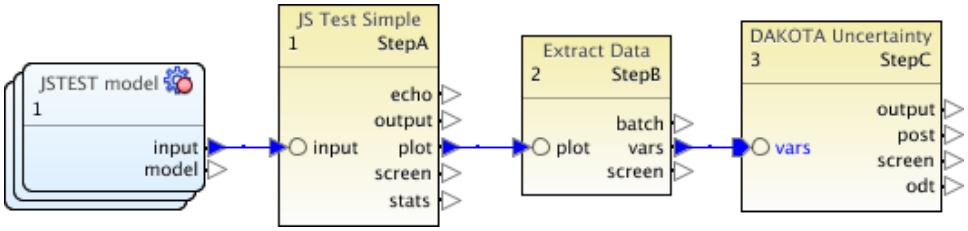


Figure 4.1. Sample Uncertainty Stream

Model nodes that represent the parametric inputs must have the **Parametric** property set to **True**. Once set, any stream steps connected to the model node, as well as all steps connected downstream, will be run once for each sample. The sequence of steps can be as simple as a single code run (such as in the sample stream figure above) or as complex as a set of multiple restarts that involves multiple analysis codes. The only requirement for the stream structure is that it includes a response extraction step (see AptPlot Data Extraction Step) connected to the output of a code step, and a DAKOTA Uncertainty "fan-in" step (see DAKOTA Uncertainty Step) connected to the output of the response extractions step.

4.1. AptPlot Data Extraction Step

The generic AptPlot Data Extraction step is used to retrieve data from any plot file format that AptPlot supports. This step bridges the gap between analysis code outputs and DAKOTA Uncertainty input. It operates by executing an AptPlot batch script to extract data from the plot file, then writing the scalar response values in an AptPlot ASCII variables file.

Once an AptPlot Data Extraction step has been added, several properties must be set to indicate how the responses are retrieved. The **Plot File Type** property on the step indicates the plot file format fed into the extraction step. Available plot file formats include:

- COBRA
- CONTAIN
- EXTDATA
- MELCOR
- NRC Databank
- PARCS
- RELAP5
- TRACE

Once the file format is specified, the **Plot File Data** property will need to indicate whether the plot file has been demultiplexed (a process in which the data is optimized for plotting) or uses a standard multiplexed plot file. After both of these properties have been set, you can connect the analysis code step's plot file output to the extract step input.

Note If you do not see your code listed here, it may use an existing format for its plot file output, such as EXTDATA. Consult the analysis code user's manual for more information.

The **AptPlot Script** property is used to specify the AptPlot batch commands used to extract response data from the plot file. Editing this property opens a batch command editor, shown in the figure.

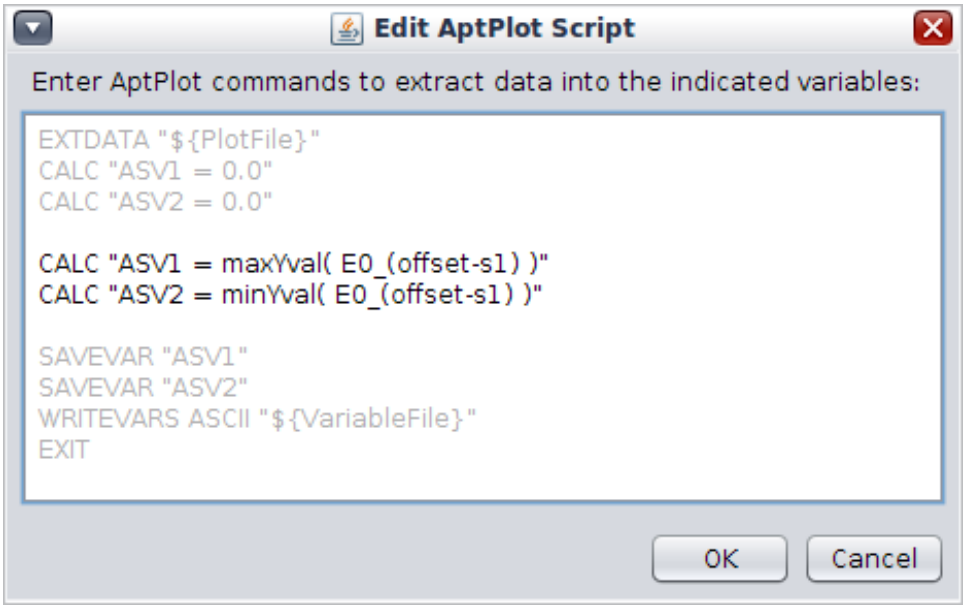


Figure 4.2. Edit Batch Script Dialog

Generated commands bookend the user-specified script; these commands cover opening the plot file, saving required scalar values (one for each figure of merit requested by the DAKOTA configuration), and writing the ASCII variable file. The generated commands cannot be modified. The remainder of the script can be edited to define how the response data is extracted from the plot file. Consult the AptPlot user's manual for more information on supported batch script commands.

Note During stream execution, the `${PlotFile}` token is automatically replaced with the path to the plot file.

Once the script is complete, press the **OK** button to confirm the changes. You can discard your modifications at any time by pressing the **Cancel** button or closing the window.

4.2. DAKOTA Uncertainty Step

The DAKOTA Uncertainty step performs the uncertainty analysis. This is a “fan-in” step: it takes a file-set produced by a set of parametric steps and runs only once. The DAKOTA

Uncertainty step, informed by the set of extracted results and a DAKOTA Wrapper XML file (packaged with the stream by the DAKOTA configuration), aggregates the response function data into a format understood by DAKOTA, executes DAKOTA in post-run mode, and organizes the results into the required locations.

The DAKOTA step also creates reports. The uncertainty plug-in generates an OpenDocument Format (ODF) report detailing the completed uncertainty analysis. Reports provide a summary of the entire analysis, documenting the configuration input to DAKOTA, analysis code execution results and the uncertainty and sensitivity results. ODF has been chosen for its freely available support (ODF can be viewed through the OpenOffice.org suite, an ODF plug-in for Microsoft Office, etc.).

Generated reports are composed of a formal listing of the DAKOTA configuration and results, as defined by the DAKOTA configuration (see Report Configuration). The generation process leverages AptPlot to generate cumulative distribution function plots of the response for inclusion in the document. Plots of the random variates may also be included. These extra plots may be defined by either a single variate-generating probability distribution, which will yield a plot of variates plotted against their iteration index, or as a pair of distributions, where the variate values for each iteration will form a complete XY coordinate.

Appendix A. Wilks Sample Computation

The Uncertainty Analysis plug-in employs a method for computing sample sizes based on the Wilks Method, described in the paper *Determination of Sample Sizes for Setting Tolerance Limits* by S. S. Wilks. The method is used to determine a number of random samplings that must be made to assure a certain degree of confidence that a given probable range of inputs have been covered. The computation has been modified slightly to account for the order of the order statistic method (see *Order Statistic Method*).

Given the probability *P*, confidence *C*, and number of figures of merit *R* (aka response functions), the algorithm for computing the samples is described by the following pseudo-code:

```
n = 0
beta = 0
while beta < C
    beta = 0
    n = n + 1
    for j in 0 to n – R
        product = innerProduct(...)
        beta = beta + product
return n
```

Where `innerProduct(...)` is defined as:

$$\frac{n!}{j!(n-j)!}\cdot p^{j}\cdot(1-P)^{n-j}$$

When the order of the order statistic (*O*) is non-zero, and d_i is the number of bounds on response function *i*, the number of response functions (*R*) is replaced by the following expression:

$$O\cdot\left(\sum_{i=1}^{R} d_i\right)$$

Appendix B. Order Statistic Method

The Order specified in the DAKOTA configuration is used to define a response matrix created for the DAKOTA Uncertainty report.

The response matrix computation takes several variables as input. It starts out with a table of response data. Each column in this table represents one figure of merit (FOM), each row represents a random sampling iteration. From there, the Order value is used to trim and sort the table based on the upper and lower limit flags for each FOM.

The process for creating the response matrix is best described by example. Consider the following table data from a hypothetical uncertainty run of twelve samples with three FOM values per iteration. In this case, we will say that the DAKOTA configuraiton specifies an order of 2, with upper and lower limit flags (T for true and F for false) as shown in the figure.

Response Data

1	6	10	8
2	3	4	10
3	11	5	11
4	7	2	6
5	8	9	9
6	5	7	4
7	1	3	5
8	2	11	1
9	4	6	7
10	9	12	3
11	10	1	2
12	12	8	12

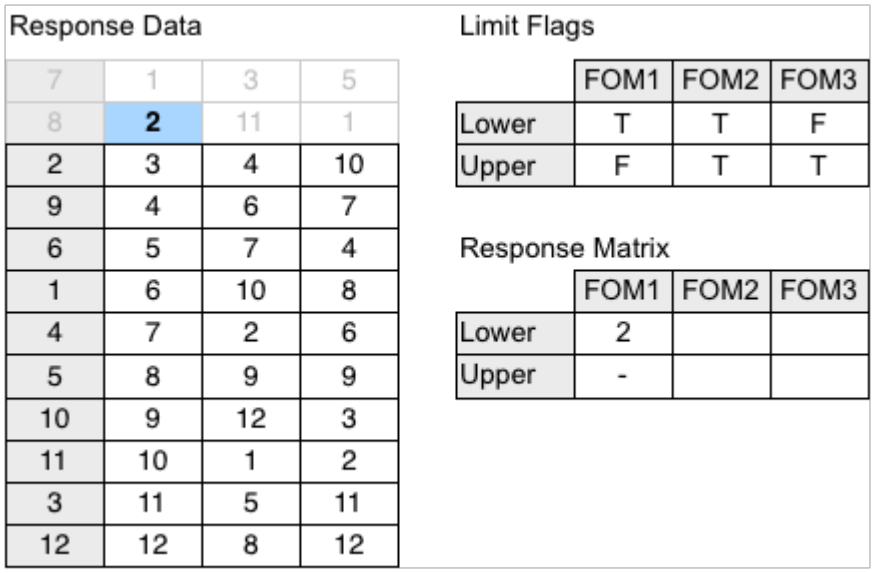
Limit Flags

	FOM1	FOM2	FOM3
Lower	T	T	F
Upper	F	T	T

Response Matrix

	FOM1	FOM2	FOM3
Lower			
Upper			

The second figure represents the table after handling FOM1. It starts by sorting table rows by values in the column for FOM1. Then, since the lower limit flag for FOM1 is set to true and the order is set to two, the top two rows in the table are removed (these rows represent the smallest values in FOM1). The number of rows removed at any step is always equal to the order value. The largest FOM1 value from the clipped rows is set as the lower value in the response matrix, and the process moves on to FOM2.



Response Data

7	1	3	5
8	**2**	11	1
2	3	4	10
9	4	6	7
6	5	7	4
1	6	10	8
4	7	2	6
5	8	9	9
10	9	12	3
11	10	1	2
3	11	5	11
12	12	8	12

Limit Flags

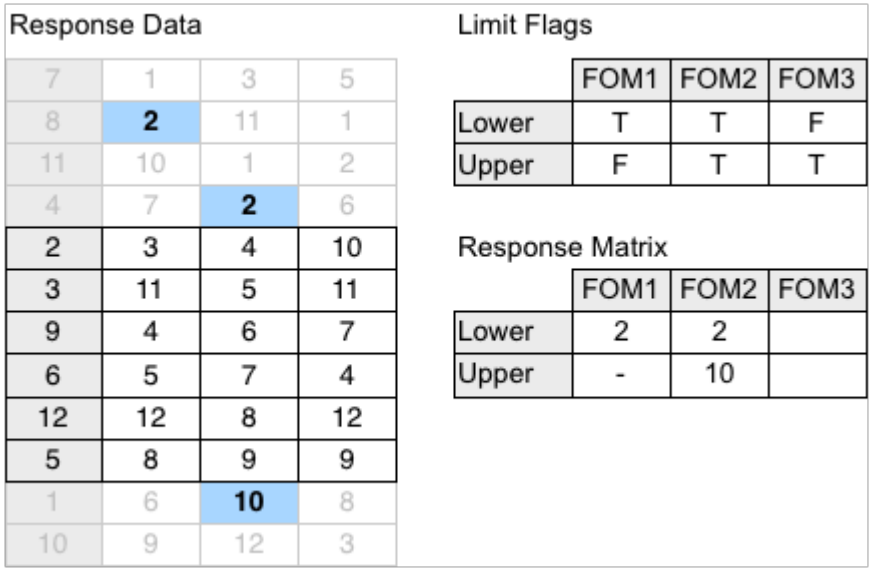
	FOM1	FOM2	FOM3
Lower	T	T	F
Upper	F	T	T

Response Matrix

	FOM1	FOM2	FOM3
Lower	2		
Upper	-		

Note An upper limit value is not defined in the response matrix for FOM1, since the upper limit flag is set to false.

The third figure represents the table after handling FOM2. Once again, it sorts the available table rows by values in the column for FOM2 (note that the two rows "removed" in the previous step did not move and are not considered). As the lower and upper limit flags for FOM2 are both set to true, two rows are removed from both the top and the bottom of the remaining data. The lower response value is once again set to the largest value from the two rows removed at the top, while the upper limit response value is taken from the smallest value from the two rows removed from at bottom. The response for FOM2 is now complete, so the process moves on to FOM3.



Response Data

7	1	3	5
8	**2**	11	1
11	10	1	2
4	7	**2**	6
2	3	4	10
3	11	5	11
9	4	6	7
6	5	7	4
12	12	8	12
5	8	9	9
1	6	**10**	8
10	9	12	3

Limit Flags

	FOM1	FOM2	FOM3
Lower	T	T	F
Upper	F	T	T

Response Matrix

	FOM1	FOM2	FOM3
Lower	2	2	
Upper	-	10	

The remaining table data is sorted on the FOM3 column. This time, the FOM1 lower limit flag is false, so the top of the table is not modified. The upper limit flag for FOM3 is set, so the bottom two rows of the available data are removed, with the smallest value set in the response matrix. The response matrix is now complete, as shown in the figure.

Response Data

7	1	3	5
8	**2**	11	1
11	10	1	2
4	7	**2**	6
6	5	7	4
9	4	6	7
5	8	9	9
2	3	4	10
3	11	5	**11**
12	12	8	12
1	6	**10**	8
10	9	12	3

Limit Flags

	FOM1	FOM2	FOM3
Lower	T	T	F
Upper	F	T	T

Response Matrix

	FOM1	FOM2	FOM3
Lower	2	2	-
Upper	-	10	11

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